Syllabus

PHYS5v48 - Computational Biophysics **Fall 2023**

Instructor: G. Andrés Cisneros, SCI 2.168
e-mail: andres@utdallas.edu
Lectures: Mon, Wed 11:30 PM – 12:45 PM
Sciences Building Computing Lab
Office Hours: Wed 10:00 – 11:00 AM or by appointment, all virtual

The course will consist of lectures and hands-on computational labs. There will be **one midterm (worth 30%)**, **computational assignments (35%)**, and a major **computational project (35%).** Midway through the semester you will submit a proposal for a final project. **The computational assignments are due two weeks after being posted**. You should start thinking about your project as early as possible and discuss it with Prof. Cisneros. You will be expected to develop a proposal for the project with minimal guidance and to develop and carry out the simulations and analysis with modest guidance when required. **The project will be individual and will involve a unique research question that may be related, or complementary of your graduate research, or commensurate with graduate-level research.**

Grading: At the end of the semester each student will receive a numerical grade that reflects their weighted scores on exams, assignments and project. Unless otherwise announced, no other factors enter into this numerical grade. Initial assignment of letter grades follows the usual break points (A = 90% and above, B = 80 to 89.99%, C = 70 to 79.99%, D = 60 to 69.99%, F = less than 60%). While some flexibility may be applied in assigning break points, this should not be assumed.

Learning outcomes

The course will provide the foundations for the application of computational simulations based on physical concepts to investigate and understand biological systems at the molecular level. The topics covered will involve material from various areas of physics, with a major emphasis on classical mechanics and molecular quantum mechanics. Students should have a working understanding of quantum and classical mechanics, electrostatics and magnetism, as well as linear algebra and calculus. No prior knowledge of biology or biochemistry is required, only a commitment to learning fundamental principles and an alternative approach for thinking of complex systems. . The emphasis will be on fundamental Quantum and Classical methods behind the simulation procedures and simulation methods. At the completion of the course the students will:

1) Understand and perform molecular simulations with Quantum Mechanics methods
2) Understand and perform molecular simulations with Molecular Mechanics methods
3) Perform calculations on small molecules and biomolecules
4) Understand force fields and basis sets
5) Be able to perform molecular parametrizations for atomistic simulations
6) Become familiar with high performance computing (HPC) environments.

Suggested Readings:

-"Molecular Modeling; Principles and Applications", A.R. Leach, 2nd Ed., Prentice Hall.
-"Molecular Driving Forces", K. Dill, S. Bromberg, 2nd Ed., Routledge.

INCLUSION & DIVERSITY

I value all students regardless of their background, country of origin, race, religion, ethnicity, disability status, etc., and am committed to providing a climate of excellence and inclusiveness within all aspects of the course. If there are aspects of your culture or identity that you would like to share with me as they relate to your success in this class, I am happy to meet to discuss. Likewise, if you have any concerns in this area or facing any special issues or challenges, you are encouraged to discuss the matter with me (set up a meeting by email) with an assurance of full confidentiality (only exception being mandatory reporting of academic integrity/code violations, and/or sexual harassment).

Tentative Schedule:

Week 1, Aug 21, 23

Introduction to the course.
Brief introduction (refresher) of biological systems (Jensen Chs. 9-10)

Week 2, Aug 28, Aug 30

Molecular quantum mechanics methods 1 (Cramer Ch. 4-8, Jensen Chs. 2-6)

Week 3, Sep. 4 ***University Holiday, No Class***, Sep. 6.

Molecular quantum mechanics methods 2 (Cramer Chs. 8-10, Jensen Chs. 9-12)

Week 4, Sep. 12, 16

Classical potentials and statistical thermodynamics (Leach Ch. 4 and 6, Dill 10, Philips 6)

Week 5, Sep 18, 20

Sampling approaches (Leach Ch. 7 and 8)

Week 6, Sep 25, 27

Water, the most anomalous solvent (Dll 30-31)

Week 7, Oct. 2, 4

Free energy methods (Leach 11)

Week 8, Oct. 9, 11

Protein Structure Prediction (Leach 10)

Proposals for term projects due

Week 9, Oct. 16, 18

Protein Simulations (Leach 9)

Midterm 10/20.

Week 10, Oct. 23, 25

Protein Simulations (Leach 9)

Week 11, Oct. 30, Nov. 1

Dimensionality Reduction, Network Analysis (Leach 9)

Week 12, Nov. 6, 8

Markov State Models

Week 13, Nov. 13, 15

QM/MM (Cramer Chp. 13)

Week 14, Nov. 20, 22 ***University Holiday, No Class all week***

Finish working on term projects

Week 15, Nov. 27, 29

Finish working on term projects during class time in computer lab with instructor

Week 16, Dec 4, 6

Finish working on term projects during class time in computer lab with instructor

Week 16, Dec 11, 13

Finals Week

Presentations of term projects during scheduled day of final

General Notes

Face Coverings

The North Texas region is currently experiencing high transmission of highly contagious and dangerous Omicron variants of COVID-19. The University of Texas at Dallas is very concerned about the risks of this new variant. UTD is requesting that all students, faculty and staff, whether vaccinated or not, comply with the public health recommendations of the U.S. Centers for Disease Control & Prevention in order to prevent Delta from spreading on campus. I ask that all students wear a mask during class and in other indoor locations on campus until we receive guidance that the public health risks have decreased significantly and no longer pose a threat. Masks will help us achieve our goal of protecting vulnerable members of the community and their families, including unvaccinated children, during this latest resurgence of COVID-19.

Read more about CDC guidelines for vaccinated people here:
https://www.cdc.gov/coronavirus/2019-ncov/vaccines/fully-vaccinated-guidance.html

Face covering guidelines could change based on community health conditions.

Attendance

Students are expected to attend class meetings regularly and to abide by the attendance policy established for the course. It is important that you communicate with the professor and the instructional team prior to being absent, so you, the professor, and the instructional team can discuss and mitigate the impact of the absence on your attainment of course learning goals. Please inform the professor and instructional team if you are unable to attend class meetings because you are ill, in mindfulness of the health and safety of everyone in our community.

If you are experiencing any symptoms of COVID-19 (https://www.cdc.gov/coronavirus/2019-ncov/symptoms-testing/symptoms.html) please seek medical attention from the Student Health Center or your health care provider PRIOR to coming to campus.

Course Materials for Remote Instruction

Remote instruction may be necessary if community health conditions change or you need to self-isolate or quarantine due to COVID-19. Students will need access to a webcam and microphone to participate in fully remote portions of the class.

Student Conduct & Discipline

The University of Texas System and The University of Texas at Dallas have rules and regulations for the orderly and efficient conduct of their business. It is the responsibility of each student and each student organization to be knowledgeable about the rules and regulations which govern student conduct and activities. General information on student conduct and discipline is contained in the UTD publication, *A to Z Guide*, which is provided to all registered students each academic year.

The University of Texas at Dallas administers student discipline within the procedures of recognized and established due process. Procedures are defined and described in the *Rules and Regulations, Board of Regents, The University of Texas System, Part 1, Chapter VI, Section 3*, and in Title V, Rules on Student Services and Activities of the university's *Handbook of Operating Procedures*. Copies of these rules and regulations are available to students in the Office of the Dean of Students, where staff members are available to assist students in interpreting the rules and regulations (SU 1.602, 972/883-6391).

A student at the university neither loses the rights nor escapes the responsibilities of citizenship. He or she is expected to obey federal, state, and local laws as well as the Regents' Rules, university regulations, and administrative rules. Students are subject to discipline for violating the standards of conduct whether such conduct takes place on or off campus, or whether civil or criminal penalties are also imposed for such conduct.

Religious Holy Days

The University of Texas at Dallas will excuse a student from class or other required activities for the travel to and observance of a religious holy day for a religion whose places of worship are exempt from property tax under Section 11.20, Tax Code, Texas Code Annotated.

The student is encouraged to notify the instructor or activity sponsor as soon as possible regarding the absence, preferably in advance of the assignment. The student, so excused, will be allowed to take the exam or complete the assignment within a reasonable time after the absence: a period equal to the length of the absence, up to a maximum of one week. A student who notifies the instructor and completes any missed exam or assignment may not be penalized for the absence. A student who fails to complete the exam or assignment within the prescribed period may receive a failing grade for that exam or assignment.

If a student or an instructor disagrees about the nature of the absence [i.e., for the purpose of observing a religious holy day] or if there is similar disagreement about whether the student has been given a reasonable time to complete any missed assignments or examinations, either the student or the instructor may request a ruling from the chief executive officer of the institution, or his or her designee. The chief executive officer or designee must take into account the legislative intent of TEC 51.911(b), and the student and instructor will abide by the decision of the chief executive officer or designee.

Academic Dishonesty -- Plagiarism and Cheating

Academic misbehavior means any activity that tends to compromise the academic integrity of the institution or subvert the education process. All forms of academic misbehavior are prohibited at the University of Texas at Dallas, as outlined in the Student Code of Conduct (https://policy.utdallas.edu/utdsp5003). Students who commit or assist in committing dishonest acts are subject to **downgrading** (to a failing grade for the test, paper, or other course-related activity in question, or for the entire course) and/or **additional sanctions** as described in the Student Code of Conduct.

Cheating: Intentionally using or attempting to use, or intentionally providing or attempting to provide, unauthorized materials, information or assistance in any academic exercise. Examples include: (a) copying from another student's test paper; (b) allowing another student to copy from a test paper; (c) using unauthorized material such as a "cheat sheet" during an exam.

Fabrication: Intentional and unauthorized falsification of any information or citation. Examples include: (a) citation of information not taken from the source indicated; (b) listing sources in a bibliography not used in a research paper.

Plagiarism: To take and use another's words or ideas as one's own. Examples include: (a) failure to use appropriate referencing when using the words or ideas of other persons; (b) altering the language, paraphrasing, omitting, rearranging, or forming new combinations of words in an attempt to make the thoughts of another appear as your own.

Other forms of academic misbehavior include, but are not limited to: (a) unauthorized use of resources, or any attempt to limit another student's access to educational resources, or any attempt to alter equipment

so as to lead to an incorrect answer for subsequent users; (b) enlisting the assistance of a substitute in the taking of examinations; (c) violating course rules as defined in the course syllabus or other written information provided to the student; (d) selling, buying or stealing all or part of an un-administered test or answers to the test; (e) changing or altering a grade on a test or other academic grade records.

The faculty expects from its students a high level of responsibility and academic honesty. Because the value of an academic degree depends upon the absolute integrity of the work done by the student for that degree, it is imperative that a student demonstrate a high standard of individual honor in his or her scholastic work.

Social Media Policies: Please see the document on the Blackboard site for this course (under "content")

Legal Notice Regarding Lecture Notes

My lectures and notes are protected by state common law and federal copyright law. You are authorized to take notes in class thereby creating a derivative work from my lecture, but the authorization extends only to making one set of notes for your own personal use and no other use. You are not authorized to record my lectures, to provide your notes to anyone else (hard copy or electronic), or to make any other use of those notes without express prior written permission from me.

Email Use

The University of Texas at Dallas recognizes the value and efficiency of communication between faculty/staff and students through electronic mail. At the same time, email raises some issues concerning security and the identity of each individual in an email exchange. The university encourages all official student email correspondence be sent only to a student's U.T. Dallas email address and that faculty and staff consider email from students official only if it originates from a UTD student account. This allows the university to maintain a high degree of confidence in the identity of all individual corresponding and the security of the transmitted information. UTD furnishes each student with a free email account that is to be used in all communication with university personnel. The Department of Information Resources at U.T. Dallas provides a method for students to have their U.T. Dallas mail forwarded to other accounts. My policy in this class is to **not** communicate any details regarding your grade through email. I will only discuss these details in person with a student.

Withdrawal from Class

The administration of this institution has set deadlines for withdrawal of any college-level courses. These dates and times are published in that semester's course catalog. Administration procedures must be followed. It is the student's responsibility to handle withdrawal requirements from any class. In other words, I cannot drop or withdraw any student. You must do the proper paperwork to ensure that you will not receive a final grade of "F" in a course if you choose not to attend the class once you are enrolled.

- **Last day to add/swap is Aug. 29**

Incomplete Grade Policy

As per university policy, incomplete grades will be granted only for work unavoidably missed at the semester's end and only if 70% of the course work has been completed. An incomplete grade must be resolved within eight (8) weeks from the first day of the subsequent long semester. If the required work to complete the course and to remove the incomplete grade is not submitted by the specified deadline, the incomplete grade is changed automatically to a grade of **F**.

Acceptable Student Behavior

Student behavior that interferes with an instructor's ability to conduct a class or other students' opportunity to learn is unacceptable and disruptive and will not be tolerated in any instructional forum at UTD. Students engaging in unacceptable behavior will be directed to leave the classroom and the instructor may refer the student to the Dean of Students to consider whether the student's conduct violated the Code of Student Conduct. The university's expectations for student conduct apply to all instructional forums, including university and electronic classroom, labs, discussion groups, field trips, etc. The Code of Student Conduct can be found at https://conduct.utdallas.edu/handbook/.

Retention of Student Records

Student records pertaining to this course are maintained in a secure location by the instructor of record. All records such as exams, answer sheets (with keys), and written papers submitted during the duration of the course are kept for at least one calendar year after course completion. Course work completed via the Blackboard online system, including grading information and comments, is also stored in a safe electronic environment for one year. You have a right to view your individual record; however, information about your records will not be divulged to other individuals without the proper written consent. You are encouraged to review the Public Information Policy and the Family Educational Rights and Privacy Act (FERPA) laws and the university's policy in accordance with those mandates at the following link: https://registrar.utdallas.edu/legislative-policies/ferpa/

Universal Evaluation System Class Evaluation

Student feedback is important and an essential part of participation in this course. The UES Class evaluation is a requirement for all organized classes at UTD. This short survey will be made available at the end of the semester to provide you with an opportunity to evaluate how this course is taught.

Disability Services

The goal of Disability Services is to provide students with disabilities educational opportunities equal to those of their non-disabled peers. Disability Services is located in room 1.610 in the Student Union. Office hours are Monday and Thursday, 8:30 a.m. to 6:30 p.m.; Tuesday and Wednesday, 8:30 a.m. to 7:30 p.m.; and Friday, 8:30 a.m. to 5:30 p.m. The contact information for the Office of Disability Services is:
The University of Texas at Dallas, SU 22
PO Box 830688
Richardson, Texas 75083-0688
(972) 883-2098 (voice or TTY)

Essentially, the law requires that colleges and universities make those reasonable adjustments necessary to eliminate discrimination on the basis of disability. For example, it may be necessary to remove classroom prohibitions against tape recorders or animals (in the case of dog guides) for students who are blind. Occasionally an assignment requirement may be substituted (for example, a research paper versus an oral presentation for a student who is hearing impaired). Classes enrolled students with mobility impairments may have to be rescheduled in accessible facilities. The college or university may need to provide special services such as registration, note-taking, or mobility assistance.
It is the student's responsibility to notify his or her professors of the need for such an accommodation. Disability Services provides students with letters to present to faculty members to verify that the student has a disability and needs accommodations. Individuals requiring special accommodation should contact the professor after class or during office hours.

Off-Campus Instruction and Course Activities

Off-campus, out-of-state, and foreign instruction and activities are subject to state law and University policies and procedures regarding travel and risk-related activities. Information regarding these rules and regulations may be found at the website address given below. Additional information is available from the office of the school dean.
(http://www.utdallas.edu/Business Affairs/Travel_Risk_Activities.htm)

These descriptions and timelines are subject to change at the discretion of the Professor.